

Nonylphenyl diphenyl phosphate, mixed isomers  
64532-97-4 | DTXSID4025797

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $4.71 \times 10^{-11}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Outside

**Local applicability domain index:**  $5.37 \times 10^{-2}$

**Confidence level:**  $6.97 \times 10^{-1}$

## Nearest Neighbors from the Training Set

Image not found

1,4-Benzoquinone

**Measured:**  $4.60 \times 10^{-12}$

**Predicted:**  $5.97 \times 10^{-12}$

Image not found

1,3,5-Cycloheptatriene

**Measured:**  $9.69 \times 10^{-11}$

**Predicted:**  $1.00 \times 10^{-10}$